

Departments of Computer Science, Mathematics, Statistics, and the Computation Institute

SCIENTIFIC AND STATISTICAL COMPUTING SEMINAR

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If the Multiparticle Schrödinger Equation Were Easy to Solve, then Chemistry Would Be Too Boring to Support Life.

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Eckhart 133, 5734 S. University Avenue

ABSTRACT

The multiparticle Schrödinger equation is the basic governing equation in quantum mechanics. Many person-centuries and cpu-millennia have been spent constructing approximate solutions to it. We should be glad it is so hard to solve because its subtle behavior allows the rich Chemistry upon which life depends.

I will describe the multiparticle Schrödinger equation and explain (some of) the reasons it is difficult to solve: high-dimensionality, antisymmetry, scaling to large systems, interparticle cusps, singular potentials and nuclear cusps, odd function spaces, etc. I will also describe our efforts to overcome these difficulties

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